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On the reaction path concept of Olender and Elber. (English)

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Summary: The Olender-Elber (OE) reaction path concept [*R. Olender* and *R. Elber*, J. Mol. Struct. 63, 398-399 (1997)] is shown to be unrelated, in general, with a true steepest descent path (SDP) in the mathematical sense yet the solutions of such a variational problem may even replace the old reaction path (RP) concept if the RP passes through several critical points of the potential energy surface. We have found a chemically interesting and sufficient condition for the coincidence of OE's "SDP" and the IRC of *K. Fukui* [J. Phys. Chem. 74, 4161 ff (1970)]. The OE concept has been discussed here in a rather straightforward manner giving it an exact mathematical description.

Keywords : reaction path; potential energy surface; steepest descent path

Classification :

*92E20 Chemical flows, reactions, etc.